Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,2-Bis(2-hydroxy-5-methylbenzylidene)-hydrazine

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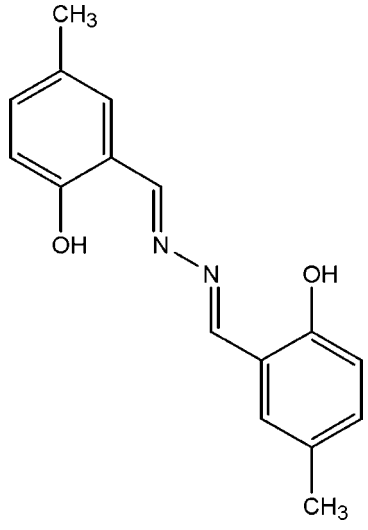
Received 27 July 2013; accepted 1 August 2013

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.154; data-to-parameter ratio = 16.0.

The molecular structure of the title compound, $C_{16}H_{16}N_2O_2$, is stabilized by intramolecular O—H···N hydrogen bonds with S(6) graph-set motifs, so that the molecule is almost planar, with a C=N—N=C torsion angle of −179.7 (2)° and a dihedral angle of 1.82 (12)° between the aromatic rings. In the crystal, weak C—H···π interactions lead to the formation of a three-dimensional network.

Related literature

For the biological activity of Schiff base ligands, see: Kelley *et al.* (1995); Pandeya *et al.* (1999); Singh & Dash (1988); Tarafder *et al.* (2002). For standard bond lengths, see: Allen *et al.* (1987). For related strucutures, see: Chantrapromma *et al.* (2010); Fun *et al.* (2010). For graph-set motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{16}H_{16}N_2O_2$
M_r = 268.31
Orthorhombic, $P2_12_12_1$
a = 6.0108 (5) Å
b = 7.3394 (5) Å
c = 31.674 (2) Å
V = 1397.32 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.22 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.987
5699 measured reflections
2952 independent reflections
1780 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.154
S = 1.02
2952 reflections
185 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C10–C15 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*A*···N2	0.82	1.91	2.635 (3)	146
O1—H1···N1	0.82	1.93	2.646 (3)	145
C5—H5···*Cg*1^{i}	0.93	2.84	3.519 (3)	130
C14—H14···*Cg*2^{ii}	0.93	2.85	3.519 (3)	130

Symmetry codes: (i) $-x-1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{5}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge the Department of Chemistry, IIT Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5296).

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supplementary materials

Acta Cryst. (2013). E**69**, o1394–o1395 [doi:10.1107/S160053681302148X]

1,2-Bis(2-hydroxy-5-methylbenzylidene)hydrazine

B. Saravanan, A. Jayamani, N. Sengottuvelan, G. Chakkaravarthi and V. Manivannan

1. Comment

Schiff base ligands exhibit anti-cancer, anti-fungal, anti-tumour and anti-HIV activities (Pandeya *et al.*, 1999; Singh & Dash, 1988; Kelley *et al.*, 1995; Tarafder *et al.*, 2002). In the molecular structure of the title compound (Fig. 1), the bond distances are within the normal range (Allen *et al.*, 1987) and are comparable with the related structures (Chantrapromma *et al.*, 2010; Fun *et al.*, 2010). In the molecule, two aromatic rings are almost co-planar, with a dihedral angle of 1.82 (12)°. The hydroxy groups form intramolecular O—H···N hydrogen bonds (O1—H1···N1 and O2—H2A···N2; Table 1) with S(6) graph-set motifs (Bernstein *et al.*, 1995). The crystal structure also exhibits weak intermolecular C—H···π (Table 1) interactions which forms a three dimensional network.

2. Experimental

The title compound was synthesized by mixing a solution (1:2 molar ratio) of hydrazine hydrate (0.20 ml, 4 mmol) and 2-hydroxy-5-methylbenzaldehyde (1.08 g, 8 mmol) in ethanol (30 ml). The resulting solution was refluxed for 4 h, yielding (65%) the pale yellow crystalline solid. The resultant solid was filtered off and washed with methanol. Pale Yellow single crystals of the title compound suitable for X-ray structure determination were recrystalized from dimethylformamide by slow evaporation at room temperature over several days.

3. Refinement

H atoms were positioned geometrically with C—H = 0.93–0.96 Å and O—H = 0.82 Å and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O, methyl C).

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

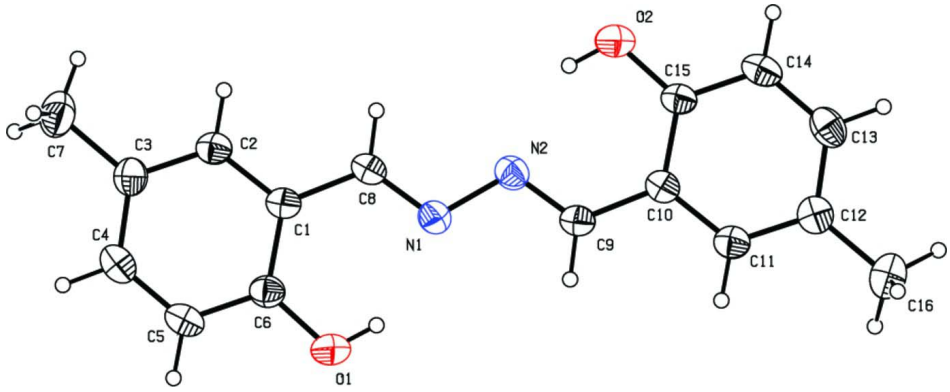

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

2-{[2-(2-Hydroxy-5-methylbenzylidene)hydrazin-1-ylidene]methyl}-4-methylphenol

Crystal data

$C_{16}H_{16}N_2O_2$
$M_r = 268.31$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.0108$ (5) Å
$b = 7.3394$ (5) Å
$c = 31.674$ (2) Å
$V = 1397.32$ (17) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.275$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2658 reflections
$\theta = 2.4$–$27.2°$
$\mu = 0.09$ mm^{-1}
$T = 295$ K
Block, yellow
0.22 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.982$, $T_{max} = 0.987$
5699 measured reflections
2952 independent reflections
1780 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.2°$, $\theta_{min} = 2.6°$
$h = -6 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -40 \rightarrow 39$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.154$
$S = 1.02$
2952 reflections
185 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0788P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.1393 (4)	0.8872 (3)	0.28106 (7)	0.0424 (6)
C2	−0.0535 (4)	0.9211 (3)	0.24097 (7)	0.0467 (6)
H2	0.0874	0.9726	0.2387	0.056*
C3	−0.1689 (5)	0.8812 (4)	0.20427 (8)	0.0528 (7)
C4	−0.3790 (5)	0.8051 (4)	0.20879 (8)	0.0558 (7)
H4	−0.4604	0.7765	0.1847	0.067*
C5	−0.4700 (5)	0.7708 (3)	0.24753 (9)	0.0540 (7)
H5	−0.6106	0.7185	0.2493	0.065*
C6	−0.3559 (4)	0.8129 (4)	0.28389 (8)	0.0474 (7)
C7	−0.0682 (6)	0.9219 (4)	0.16150 (7)	0.0766 (10)
H7A	−0.0947	0.8212	0.1428	0.115*
H7B	0.0891	0.9405	0.1645	0.115*
H7C	−0.1352	1.0299	0.1500	0.115*
C8	−0.0071 (4)	0.9275 (3)	0.31799 (7)	0.0454 (6)
H8	0.1363	0.9726	0.3145	0.055*
C9	−0.0019 (4)	0.9213 (3)	0.42464 (7)	0.0451 (6)
H9	−0.1451	0.8758	0.4282	0.054*
C10	0.1302 (5)	0.9612 (3)	0.46142 (7)	0.0429 (6)
C11	0.0395 (5)	0.9322 (3)	0.50158 (7)	0.0478 (7)
H11	−0.1016	0.8810	0.5035	0.057*
C12	0.1501 (5)	0.9762 (3)	0.53841 (8)	0.0527 (7)
C13	0.3625 (6)	1.0501 (4)	0.53396 (8)	0.0578 (8)
H13	0.4417	1.0814	0.5581	0.069*
C14	0.4593 (5)	1.0786 (4)	0.49519 (8)	0.0556 (7)
H14	0.6019	1.1271	0.4935	0.067*
C15	0.3451 (5)	1.0352 (3)	0.45871 (8)	0.0460 (6)
C16	0.0438 (6)	0.9530 (4)	0.58087 (8)	0.0718 (9)
H16A	−0.0435	1.0588	0.5874	0.108*
H16B	0.1573	0.9378	0.6019	0.108*
H16C	−0.0504	0.8474	0.5805	0.108*
N1	−0.0818 (3)	0.9027 (3)	0.35543 (6)	0.0498 (6)
N2	0.0716 (4)	0.9465 (3)	0.38727 (6)	0.0498 (6)
O1	−0.4551 (3)	0.7801 (3)	0.32150 (5)	0.0680 (6)
H1	−0.3751	0.8171	0.3406	0.102*
O2	0.4451 (3)	1.0657 (3)	0.42094 (6)	0.0650 (6)
H2A	0.3623	1.0328	0.4018	0.098*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0381 (15)	0.0357 (12)	0.0534 (14)	0.0023 (12)	−0.0003 (12)	0.0034 (10)
C2	0.0442 (15)	0.0392 (13)	0.0565 (16)	0.0000 (13)	−0.0007 (12)	0.0069 (11)
C3	0.0594 (19)	0.0491 (15)	0.0499 (15)	0.0053 (16)	−0.0034 (13)	0.0016 (12)
C4	0.0553 (19)	0.0488 (15)	0.0633 (17)	0.0011 (16)	−0.0152 (15)	−0.0051 (13)
C5	0.0412 (15)	0.0494 (14)	0.0715 (17)	−0.0039 (14)	−0.0070 (15)	−0.0016 (14)
C6	0.0417 (16)	0.0458 (14)	0.0548 (15)	0.0020 (14)	0.0002 (13)	0.0028 (11)
C7	0.102 (3)	0.076 (2)	0.0512 (16)	−0.006 (2)	−0.0028 (17)	0.0065 (14)
C8	0.0386 (16)	0.0415 (13)	0.0562 (15)	−0.0024 (13)	−0.0057 (12)	0.0003 (12)
C9	0.0395 (15)	0.0413 (13)	0.0546 (14)	−0.0010 (13)	0.0000 (12)	0.0035 (11)
C10	0.0412 (17)	0.0358 (12)	0.0518 (14)	0.0041 (12)	−0.0031 (12)	0.0002 (10)
C11	0.0465 (17)	0.0399 (13)	0.0570 (15)	0.0003 (13)	−0.0003 (13)	0.0042 (12)
C12	0.058 (2)	0.0425 (14)	0.0572 (16)	0.0059 (15)	−0.0035 (14)	0.0008 (12)
C13	0.061 (2)	0.0471 (15)	0.0656 (18)	0.0036 (16)	−0.0186 (15)	−0.0005 (13)
C14	0.0401 (17)	0.0508 (15)	0.0759 (19)	−0.0037 (15)	−0.0086 (14)	0.0047 (14)
C15	0.0379 (16)	0.0436 (14)	0.0564 (15)	−0.0008 (13)	−0.0007 (13)	0.0036 (12)
C16	0.091 (3)	0.0697 (18)	0.0550 (16)	0.005 (2)	0.0022 (17)	0.0006 (14)
N1	0.0458 (13)	0.0551 (13)	0.0485 (11)	−0.0018 (12)	−0.0044 (10)	0.0023 (10)
N2	0.0476 (13)	0.0490 (12)	0.0527 (11)	−0.0004 (11)	−0.0053 (11)	0.0021 (9)
O1	0.0460 (12)	0.0922 (16)	0.0658 (12)	−0.0134 (12)	0.0067 (10)	0.0055 (12)
O2	0.0490 (12)	0.0778 (14)	0.0683 (11)	−0.0112 (12)	0.0037 (10)	0.0053 (11)

Geometric parameters (Å, º)

C1—C2	1.393 (3)	C9—H9	0.9300
C1—C6	1.415 (3)	C10—C11	1.400 (3)
C1—C8	1.445 (3)	C10—C15	1.404 (3)
C2—C3	1.385 (3)	C11—C12	1.381 (3)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.388 (4)	C12—C13	1.395 (4)
C3—C7	1.514 (3)	C12—C16	1.499 (3)
C4—C5	1.367 (4)	C13—C14	1.375 (4)
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.376 (3)	C14—C15	1.381 (3)
C5—H5	0.9300	C14—H14	0.9300
C6—O1	1.354 (3)	C15—O2	1.357 (3)
C7—H7A	0.9600	C16—H16A	0.9600
C7—H7B	0.9600	C16—H16B	0.9600
C7—H7C	0.9600	C16—H16C	0.9600
C8—N1	1.281 (3)	N1—N2	1.404 (3)
C8—H8	0.9300	O1—H1	0.8200
C9—N2	1.277 (3)	O2—H2A	0.8200
C9—C10	1.440 (3)		
C2—C1—C6	117.9 (2)	C10—C9—H9	119.0
C2—C1—C8	119.9 (2)	C11—C10—C15	118.2 (2)
C6—C1—C8	122.3 (2)	C11—C10—C9	119.3 (3)
C3—C2—C1	122.8 (2)	C15—C10—C9	122.5 (2)

C3—C2—H2	118.6	C12—C11—C10	123.0 (3)
C1—C2—H2	118.6	C12—C11—H11	118.5
C2—C3—C4	117.0 (2)	C10—C11—H11	118.5
C2—C3—C7	120.6 (3)	C11—C12—C13	116.5 (3)
C4—C3—C7	122.4 (3)	C11—C12—C16	121.8 (3)
C5—C4—C3	122.0 (3)	C13—C12—C16	121.7 (3)
C5—C4—H4	119.0	C14—C13—C12	122.5 (3)
C3—C4—H4	119.0	C14—C13—H13	118.8
C4—C5—C6	120.7 (3)	C12—C13—H13	118.8
C4—C5—H5	119.6	C13—C14—C15	120.1 (3)
C6—C5—H5	119.6	C13—C14—H14	119.9
O1—C6—C5	118.5 (2)	C15—C14—H14	119.9
O1—C6—C1	122.0 (2)	O2—C15—C14	118.6 (3)
C5—C6—C1	119.5 (2)	O2—C15—C10	121.7 (2)
C3—C7—H7A	109.5	C14—C15—C10	119.7 (2)
C3—C7—H7B	109.5	C12—C16—H16A	109.5
H7A—C7—H7B	109.5	C12—C16—H16B	109.5
C3—C7—H7C	109.5	H16A—C16—H16B	109.5
H7A—C7—H7C	109.5	C12—C16—H16C	109.5
H7B—C7—H7C	109.5	H16A—C16—H16C	109.5
N1—C8—C1	121.8 (2)	H16B—C16—H16C	109.5
N1—C8—H8	119.1	C8—N1—N2	113.7 (2)
C1—C8—H8	119.1	C9—N2—N1	113.9 (2)
N2—C9—C10	122.0 (2)	C6—O1—H1	109.5
N2—C9—H9	119.0	C15—O2—H2A	109.5
C6—C1—C2—C3	−1.5 (4)	C15—C10—C11—C12	1.3 (4)
C8—C1—C2—C3	178.2 (2)	C9—C10—C11—C12	−176.3 (2)
C1—C2—C3—C4	0.3 (4)	C10—C11—C12—C13	−0.9 (4)
C1—C2—C3—C7	179.6 (2)	C10—C11—C12—C16	176.6 (2)
C2—C3—C4—C5	0.2 (4)	C11—C12—C13—C14	0.0 (4)
C7—C3—C4—C5	−179.1 (3)	C16—C12—C13—C14	−177.6 (2)
C3—C4—C5—C6	0.7 (4)	C12—C13—C14—C15	0.6 (4)
C4—C5—C6—O1	178.5 (2)	C13—C14—C15—O2	179.7 (2)
C4—C5—C6—C1	−1.9 (4)	C13—C14—C15—C10	−0.3 (4)
C2—C1—C6—O1	−178.2 (2)	C11—C10—C15—O2	179.4 (2)
C8—C1—C6—O1	2.1 (4)	C9—C10—C15—O2	−3.1 (4)
C2—C1—C6—C5	2.3 (4)	C11—C10—C15—C14	−0.6 (3)
C8—C1—C6—C5	−177.4 (2)	C9—C10—C15—C14	176.9 (2)
C2—C1—C8—N1	178.2 (2)	C1—C8—N1—N2	179.0 (2)
C6—C1—C8—N1	−2.0 (4)	C10—C9—N2—N1	−179.07 (19)
N2—C9—C10—C11	179.4 (2)	C8—N1—N2—C9	−179.7 (2)
N2—C9—C10—C15	2.0 (4)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C10–C15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N2	0.82	1.91	2.635 (3)	146
O1—H1···N1	0.82	1.93	2.646 (3)	145

C5—H5···*Cg*1^{i}	0.93	2.84	3.519 (3)	130
C14—H14···*Cg*2^{ii}	0.93	2.85	3.519 (3)	130

Symmetry codes: (i) −*x*−1, *y*−1/2, −*z*+1/2; (ii) *x*+1/2, −*y*+5/2, −*z*+1.